REPORT DOCUMENTATION PAGE AFRL-SR-BL-TR-00-Public reporting burden for this collection of information is estimated to average 1 hour per response, gathering and maintaining the data needed, and completing and reviewing the collection of information. including suggestions for reducing this burden, to Washington Headquarters: Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of the Office of Management and Budget, Paperwirk Reducing the Control of the Office of th data sources, aspect of this 1215 Jefferson 0651 3. REPORT TYPE AND DATES COVERED 1. AGENCY USE ONLY (Leave Blank) 2. REPORT DATE August 30, 2000 Final Report 01/01/97 - 04/30/2000TITLE AND SUBTITLE 5. FUNDING NUMBERS A Pareto Framework for Bayesian-Validated Computer-Simulation F49620-97-1-0052 Surrogates 6. AUTHORS Anthony T. Patera, Dimitrios Royas, Luc Machiels, and Yvon Maday 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) 8. PERFORMING ORGANIZATION REPORT NUMBER Massachusetts Institute of Technology Department of Mechanical Engineering; Room 3-266 77 Massachusetts Avenue Cambridge, MA 02139-4307 SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) SPONSORING / MONITORING AGENCY REPORT NUMBER Air Force Office of Scientific Research N/A AFOSR/NM 801 North Randolph, Rm 732 Arlington, VA 22203-1977 11. SUPPLEMENTARY NOTES 12b. DISTRIBUTION CODE 12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; Distribution unlimited. 13. ABSTRACT (Maximum 200 words) In this project we have developed a two-stage off-line/on-line blackbox reduced-basis output bound method for the prediction of outputs (quantities of interest) of elliptic partial differential equations with affine parameter dependence. The computational complexity of the on-line stage of the procedure scales only with the dimension of the reduced-basis space and the parametric complexity of the partial differential operator. The method is both efficient and certain: thanks to rigorous a posteriori error bounds, we may (safely) retain only the minimal number of modes necessary to achieve the prescribed accuracy in the output of interest. The technique is particularly appropriate for applications such as design and optimization, in which repeated and rapid evaluation of the output is required. DTIC QUALITY INSPESSED 20001205 08 14. SUBJECT TERMS 15. NUMBER OF PAGES Surrogates, Reduced-Basis Methods, Output Bounds, A Posteriori Error Estimation,

OF REPORT

Partial Differential Equations

17. SECURITY CLASSIFICATION

UNCLASSIFIED

18. SECURITY CLASSIFICATION

OF THIS PAGE

UNCLASSIFIED

LIMITATION OF ABSTRACT

16. PRICE CODE

SAR

19. SECURITY CLASSIFICATION

UNCLASSIFIED

OF ABSTRACT

Reduced-Basis Output-Bound Methods for Elliptic Partial Differential Equations¹

Anthony T. Patera

Department of Mechanical Engineering, Room 3-264, Massachusetts Institute of Technology, Cambridge, MA, 02139-4307, patera@mit.edu

Dimitrios V. Rovas

Department of Mechanical Engineering, Room 3-243, Massachusetts Institute of Technology, Cambridge, MA, 02139-4307, rovas@mit.edu

Luc Machiels

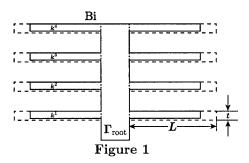
Lawrence Livermore National Laboratory, L-561, 7000 East Avenue, Livermore, CA 94550, machiels1@llnl.gov

1 Motivation

This grant has focussed on the development of new techniques for very rapid and repeated evaluation of outputs of elliptic partial differential equations. The goal is to develop methods that are sufficiently fast to permit general design and optimization studies, that is, full exploration of the design space of interest. Initially we approached the problem through "computer-simulation surrogates": input-output pair interpolations validated via statistical measures. However, these surrogates degraded very rapidly with increasing design-space dimension, both as regards their approximation properties and also in terms of the relevance of the probabilistic validation statement. We thus turned to a second approach which, because it is based on an underlying state-space representation, fares much better with increasing dimensionality; furthermore, the associated error estimates are no longer statistical, and thus much more useful in practice. In this report we motivate and explain these techniques in a particular (simple) context, and also indicate the various extensions that have been developed in order to treat a larger class of problems. This report (minus this paragraph) has also appeared recently in the SIAM SIAG/OPT newsletter Volume 11, Number 2.

To motivate and illustrate our methods we consider a specific example: a thermal fin. The fin, shown in Figure 1, consists of a central "post" and four "subfins;" the fin conducts heat from a prescribed uniform flux "source" at the root, $\Gamma_{\rm root}$, through the large-surface-area subfins to surrounding flowing air. The fin is characterized by seven design parameters, or "inputs," $\mu \in \mathcal{D} \subset \mathbb{R}^{P=7}$, where $\mu^i = k^i, i = 1, \ldots, 4, \mu^5 = \text{Bi}, \mu^6 = L$, and $\mu^7 = t$. Here k^i is the thermal conductivity of the i^{th} subfin (normalized relative to the post conductivity); Bi is the Biot number, a nondimensional heat transfer coefficient reflecting convective transport to the air at the fin surfaces; and L and t are the length and thickness of the subfins (normalized relative to the post width). The performance metric, or "output," $s \in \mathbb{R}$, is chosen to be the average temperature of the fin root normalized by the prescribed heat flux into the fin root. In order to optimize the fin design, we must be able to evaluate $s(\mu)$ repeatedly and rapidly.

¹The material presented here is work performed in collaboration with Professor Yvon Maday of University of Paris VI and reported in greater detail in references [1, 2, 3, 4].



We can express our input-output relationship as $s = \ell^O(u(\mu))$, where $\ell^O(v)$ is a (continuous) linear functional — $\ell^O(v) = \int_{\Gamma_{\text{root}}} v$ — and $u(\mu)$ is the temperature distribution within the fin. (The temperature field is of course a function of the spatial coordinate, \boldsymbol{x} ; we explicitly indicate this dependence only as needed.) The temperature distribution $u(\mu) \in Y$ satisfies the elliptic partial differential equation describing heat conduction in the fin,

$$a(u, v; \mu) = \ell(v), \forall v \in Y; \tag{1}$$

 $a(u,v;\mu)$ is the weak form of the Laplacian, and $\ell(v)$ reflects the prescribed heat flux at the root. Here Y is the appropriate Hilbert space with associated inner product $(\cdot,\cdot)_Y$ and induced norm $\|\cdot\|_Y^2$. The bilinear form $a(\cdot,\cdot;\mu)$ is symmetric, $a(w,v;\mu)=a(v,w;\mu), \forall w,v\in Y^2, \forall \mu\in\mathcal{D};$ uniformly continuous, $|a(w,v;\mu)|\leq \gamma\|w\|_Y\|v\|_Y, \forall w,v\in Y^2, \forall \mu\in\mathcal{D};$ and coercive, $\alpha\|v\|_Y^2\leq a(v,v;\mu), \forall v\in Y, \forall \mu\in\mathcal{D}.$ Here α and γ are strictly positive real constants. Finally, the form $\ell(v)$ is a linear bounded functional; for our choice of scaling and output, $\ell^O(v)=\ell(v)$, which we will exploit to simplify the exposition.

It can further be shown for our problem that a can be expressed as

$$a(w, v; \mu) = \sum_{q=1}^{Q} \sigma^{q}(\mu) a^{q}(w, v), \forall w, v \in Y^{2}, \forall \mu \in \mathcal{D},$$
 (2)

for appropriately chosen functions $\sigma^q\colon \mathcal{D}\to\mathbb{R}$ and associated μ -independent bilinear forms $a^q\colon Y\times Y\to\mathbb{R},\ q=1,\ldots,Q$. Note that we pose our problem on a fixed fin reference domain Ω in order to ensure that the parametric dependence on geometry — L and t — enters through $a(\cdot,\cdot;\mu)$ and ultimately the $\sigma^q(\mu)$. For our particular problem, Q=15; if we freeze (fix) all parameters except L and t (such that $P_{\text{eff}}=2$), Q=8; if we freeze only L and t (such that $P_{\text{eff}}=5$), Q=6.

In the context of design, optimization, and control, we require very rapid response and many output evaluations. Our goal is thus to construct an approximation to $u(\mu)$, $\tilde{u}(\mu)$, and hence approximation to $s(\mu)$, $\tilde{s}(\mu) = \ell^O(\tilde{u}(\mu))$, which

²Here $Y = H^1(\Omega)$, the space of functions that are square integrable and that have square integrable first (distributional) derivatives over the fin reference domain Ω . The inner product $(w, v)_Y$ may be chosen to be $\int_{\Omega} \nabla w \cdot \nabla v + wv$.

is (i) certifiably accurate, and (ii) very efficient in the limit of many evaluations. By the former we mean that the error in our approximate output, $|s(\mu) - \tilde{s}(\mu)|$, is guaranteed to be less than a prescribed tolerance ε ; by the latter we mean that, following an initial fixed investment, the additional incremental cost to evaluate $\tilde{s}(\mu)$ for any new $\mu \in \mathcal{D}$ is much less than the effort required to directly compute $s(\mu) = \ell^O(u(\mu))$ by (say) standard finite element approximation.

2 Reduced-Basis Approximation

Reduced-basis methods (e.g., [5, 6, 7]) are a "parameter-space" version of weighted-residual (here Galerkin) approximation. To define our reduced-basis procedure, we first introduce a sample set in parameter space, $S^N = \{\mu_1, \ldots, \mu_N\}$, and associated reduced-basis space $W^N = \text{span}\{\zeta_n \equiv u(\mu_n), n = 1, \ldots, N\}$, where $u(\mu_n)$ satisfies (1) for $\mu = \mu_n \in \mathcal{D}$ (note μ^i refers to the i^{th} component of the P-tuple μ , whereas μ_n refers to the n^{th} P-tuple in S^N). We then require our reduced-basis approximation to $u(\mu)$ for any given μ , $u^N(\mu) \in W^N \subset Y$, to satisfy

$$a(u^N(\mu), v; \mu) = \ell(v), \forall v \in W^N; \tag{3}$$

the reduced-basis approximation to $s(\mu)$ can subsequently be evaluated as $s^N(\mu) = \ell^O(u^N(\mu))$.

It is a simple matter to show that

$$||u(\mu) - u^N(\mu)||_Y \le \sqrt{\frac{\gamma}{\alpha}} \min_{w^N \in W^N} ||u(\mu) - w^N||_Y,$$
 (4)

which states that our approximation is optimal in the Y norm. It can also be readily shown for our particular problem that

$$s(\mu) = s^{N}(\mu) + a(e^{N}(\mu), e^{N}(\mu); \mu),$$
 (5)

where $e^N = u - u^N$. It follows from (4),(5), and the continuity of a that

$$|s(\mu) - s^{N}(\mu)| \le \frac{\gamma^{2}}{\alpha} (\min_{w^{N} \in W^{N}} ||u(\mu) - w^{N}||_{Y})^{2}; \tag{6}$$

thus our output approximation is also optimal.

We must, of course, also understand the extent to which the best w^N in W^N can, indeed, approximate the requisite temperature distribution. The essential point is that, although W^N clearly does not have any approximation properties for general functions in Y, simple interpolation arguments in parameter space suggest that W^N should approximate well $u(\mu)$ even for very modest N; indeed, exponential convergence is obtained in N for sufficiently smooth μ -dependence (e.g., [6, 7]). It is for this reason that, even in high-dimensional (large P) parameter spaces, reduced-basis methods continue to perform well — indeed, thanks to (6), much better than $ad\ hoc$, uncontrolled "non-state-space" fits of $(\mu, s(\mu))$ input-output pairs.

We now turn to the computational issues. We first express the reduced-basis approximation as

$$u^{N}(\boldsymbol{x};\mu) = \sum_{j=1}^{N} u_{j}^{N}(\mu)\zeta_{j}(\boldsymbol{x}) = (\underline{u}^{N}(\mu))^{T}\underline{\zeta}(\boldsymbol{x}), \tag{7}$$

and choose for test functions $v = \zeta_i(x), i = 1, ..., N$. We then insert these representations into (3) to yield the desired algebraic equations for $\underline{u}^N(\mu) \in \mathbb{R}^N$,

$$\sum_{i=1}^{N} a(\zeta_j, \zeta_i; \mu) u_j^N = \ell(\zeta_i), \quad i = 1, \dots, N.$$
 (8)

Equation (8) can be written in matrix form as

$$\underline{A}(\mu)\underline{u}^{N}(\mu) = \underline{L},\tag{9}$$

where $\underline{A}(\mu) \in \mathbb{R}^{N \times N}$ is the SPD matrix with entries $A_{i,j}(\mu) = a(\zeta_j, \zeta_i; \mu), 1 \le i, j \le N$, and $\underline{L} \in \mathbb{R}^N$ is the "load" vector with entries $L_i = \ell(\zeta_i), 1 \le i \le N$. We now invoke (2) to note that

$$A_{i,j}(\mu) = a(\zeta_j, \zeta_i; \mu) = \sum_{q=1}^{Q} \sigma^q(\mu) a^q(\zeta_j, \zeta_i)$$
$$= \sum_{q=1}^{Q} \sigma^q(\mu) A_{i,j}^q, \tag{10}$$

where the matrices $\underline{A}^q \in \mathbb{R}^{N \times N}$ are given by $A_{i,j}^q = a^q(\zeta_j, \zeta_i), 1 \leq i, j \leq N, q = 1, \ldots, Q$. The off-line/on-line decomposition is now clear. In the off-line stage, we construct the $\underline{A}^q, q = 1, \ldots, Q$. In the on-line stage, for any given μ , we first form \underline{A} from the \underline{A}^q according to (10); we next invert (9) to find $\underline{u}^N(\mu)$; and we then compute $s^N(\mu) = \ell^O(u^N(\mu)) = \ell(u^N(\mu)) = (\underline{u}^N(\mu))^T \underline{L}$. As we shall see, N will typically be O(10) for our particular problem. Thus, as required, the incremental cost to evaluate $s^N(\mu)$ for any given new μ is very small: $O(N^2Q)$ to form $\underline{A}(\mu)$; $O(N^3)$ to invert (the typically dense) $\underline{A}(\mu)$ system; and O(N) to evaluate $s^N(\mu)$ from $\underline{u}^N(\mu)$.

The above a priori results tell us only that we are doing as well as possible; it does not tell us how well we are doing. Since the error in our output is not known, the minimal number of basis functions required to satisfy the desired error tolerance can not be ascertained. As a result, either too many or too few functions are retained; the former results in computational inefficiency, the latter in unacceptable uncertainty. We thus need a posteriori error bounds as well.

3 Output Bounds

To begin, we assume that we may find a function $g(\mu): \mathcal{D} \to \mathbb{R}_+$ and a symmetric continuous coercive bilinear form $\hat{a}: Y \times Y \to \mathbb{R}$ such that

$$\underline{c}\|v\|_Y^2 \le g(\mu)\hat{a}(v,v) \le a(v,v;\mu), \forall v \in Y, \forall \mu \in \mathcal{D}, \tag{11}$$

for some real positive constant \underline{c} ; for our thermal fin problem we can readily find a $g(\mu)$ and $\hat{a}(w,v)$ such that (11) is satisfied. The procedure is then simple: we first compute $\hat{e}(\mu) \in Y$ solution of

$$g(\mu)\hat{a}(\hat{e}(\mu), v) = R(v; \mu), \forall v \in Y, \tag{12}$$

where $R(v; \mu) \equiv \ell(v) - a(u^N, v; \mu)$ is the residual; we then evaluate our bounds as

$$s_{-}^{N}(\mu) = s^{N}(\mu), \quad s_{+}^{N}(\mu) = s^{N}(\mu) + \Delta^{N}(\mu),$$
 (13)

where $\Delta^{N}(\mu)$, the bound gap, is given by

$$\Delta^{N}(\mu) = g(\mu)\hat{a}(\hat{e}(\mu), \hat{e}(\mu)). \tag{14}$$

The notion of output bounds is not restricted to reduced-basis approximations: it can also be applied within the context of finite element discretization as well as iterative solution strategies [8, 9].

We can then show that

$$s_{-}^{N}(\mu) \le s(\mu) \le s_{+}^{N}(\mu), \quad \forall N; \tag{15}$$

we thus have a *certificate of fidelity* for s^N — it is within $\Delta^N(\mu)$ of $s(\mu)$. To prove the left inequality we appeal to (5) and the coercivity of a. To demonstrate the right inequality we first note that $R(e^N(\mu); \mu) = \ell(e^N(\mu)) - a(u^N(\mu), e^N(\mu); \mu) = a(e^N(\mu), e^N(\mu); \mu)$, since $\ell(e^N(\mu)) = a(u, e^N(\mu); \mu)$ from (1) for $v = e^N(\mu)$; we next choose $v = e^N(\mu)$ in (12) to obtain $g(\mu)\hat{a}(\hat{e}(\mu), e^N(\mu)) = a(e^N(\mu), e^N(\mu); \mu)$; then from the right inequality of (11) we have

$$\begin{split} \Delta^{N}(\mu) & \equiv g(\mu)\hat{a}(\hat{e}, \hat{e}) \\ & = g(\mu)\hat{a}(\hat{e} - e^{N}, \hat{e} - e^{N}) + 2a(e^{N}, e^{N}) \\ & - g(\mu)\hat{a}(e^{N}, e^{N}) \\ & \geq g(\mu)\hat{a}(\hat{e} - e^{N}, \hat{e} - e^{N}) + a(e^{N}, e^{N}); \end{split}$$

from the left inequality of (11) we thus conclude that $\Delta^N(\mu) \geq a(e^N, e^N)$; a comparison of (5) and (13) then completes the proof.

We can now ascertain, through Δ^N , the accuracy of our output prediction, which will in turn permit us to adaptively modify our approximation until the prescribed error tolerance ε is satisfied. However, it is also critical that $\Delta^N(\mu)$ be a good error estimator; a poor estimator will encourage us to unnecessarily refine an approximation which is, in fact, adequate. To prevent the latter the effectivity $\eta^N(\mu) \equiv \Delta^N(\mu)/|s(\mu) - s^N(\mu)|$ should be order unity. For our

problem it is simple to prove that $\eta^N(\mu) \leq \gamma/\underline{c}$, independent of μ and N; in practice, effectivities are typically less than 10, which is adequate given the rapid convergence of reduced-basis approximations.

We now turn to the computational issues. From (2) and (7), (12) can be re-written as

$$\begin{split} \hat{a}(\hat{e}(\mu), v) &= \\ \frac{1}{g(\mu)} \Bigg(\ell(v) - \sum_{q=1}^{Q} \sum_{j=1}^{N} \sigma^{q}(\mu) u_{j}^{N}(\mu) a^{q}(\zeta_{j}, v) \Bigg), \\ \forall v \in Y. \end{split}$$

We thus see from simple linear superposition that $\hat{e}(\mu)$ can be expressed as

$$\hat{e}(\mu) = \frac{1}{g(\mu)} (\hat{z}_0 + \sum_{q=1}^{Q} \sum_{i=1}^{N} \sigma^q(\mu) u_j^N(\mu) \hat{z}_j^q),$$

where $\hat{z}_0 \in Y$ satisfies $\hat{a}(\hat{z}_0, v) = \ell(v), \forall v \in Y$, and $\hat{z}_j^q \in Y, j = 1, ..., N, q = 1, ..., Q$, satisfies $\hat{a}(\hat{z}_j^q, v) = -a^q(\zeta_j, v), \forall v \in Y$. It then follows that we can express $\Delta^N(\mu)$ of (14) as

$$\Delta^{N}(\mu) = \frac{1}{g(\mu)} \left[\underbrace{\hat{a}(\hat{z}_{0}, \hat{z}_{0})}_{c_{0}} + 2 \sum_{q=1}^{Q} \sum_{j=1}^{N} \sigma^{q}(\mu) u_{j}^{N}(\mu) \underbrace{\hat{a}(\hat{z}_{0}, \hat{z}_{j}^{q})}_{\Lambda_{j}^{q}} + \sum_{q=1}^{Q} \sum_{q'=1}^{Q} \sum_{j=1}^{N} \sum_{j'=1}^{N} \sigma^{q}(\mu) \sigma^{q'}(\mu) u_{j}^{N}(\mu) u_{j'}^{N}(\mu) \underbrace{\hat{a}(\hat{z}_{j}^{q}, \hat{z}_{j'}^{q'})}_{\Gamma_{jj'}^{qq'}} \right];$$
(16)

 $s_{+}^{N}(\mu)$ then directly follows from (13).

The off-line/on-line decomposition is now clear. In the off-line stage we compute \hat{z}_0 and \hat{z}_j^q , $j=1,\ldots,N, q=1,\ldots,Q$, and then the inner products c_0, Λ_j^q , and $\Gamma_{jj'}^{qq'}$ defined in (16). In the on-line stage, for any given new μ , and given $s^N(\mu)$ and $\underline{u}^N(\mu)$ as computed in the on-line stage of the output prediction process (Section 2), we evaluate $\Delta^N(\mu)$ as

$$\Delta^{N}(\mu) = \frac{1}{g(\mu)} \left[c_{0} + 2 \sum_{q=1}^{Q} \sum_{j=1}^{N} \sigma^{q}(\mu) u_{j}^{N}(\mu) \Lambda_{j}^{q} + \sum_{q=1}^{Q} \sum_{j'=1}^{Q} \sum_{j'=1}^{N} \sum_{j'=1}^{N} \sigma^{q}(\mu) \sigma^{q'}(\mu) u_{j}^{N}(\mu) u_{j'}^{N}(\mu) \Gamma_{jj'}^{qq'} \right],$$

and then evaluate $s_+^N(\mu) = s^N(\mu) + \Delta^N(\mu)$. The incremental cost to evaluate $s_+^N(\mu)$ for any given new μ is very small: $O(N^2Q^2)$.

4 Numerical Algorithm

In the simplest case we take our field and output approximations to be $\tilde{u}(\mu) = u^N(\mu)$ and $\tilde{s}(\mu) = s^N(\mu)$, respectively, for some given N, and then compute $\Delta^N(\mu)$ to assess the error. However, we can improve upon this recipe: we take $\tilde{u}(\mu) = u^{\tilde{N}}(\mu)$ and $\tilde{s}(\mu) = s^{\tilde{N}}(\mu)$, where $u^{\tilde{N}}(\mu)$ and $s^{\tilde{N}}(\mu)$ are the reduced-basis approximations associated with a subspace of W^N , $W^{\tilde{N}}$, in which we select only \tilde{N} of our available basis functions. In practice, we include in $W^{\tilde{N}}$ the basis functions corresponding to sample points μ_n closest to the new μ of interest; we continue to (say) double our space until $\Delta^{\tilde{N}}(\mu) \leq \varepsilon$ (and hence $|s(\mu) - s^{\tilde{N}}(\mu)| \leq \varepsilon$). If we satisfy our criterion for $\tilde{N} \leq N$ the adaptive procedure is entirely contained within the on-line stage of the procedure, and the complexity of this stage is reduced from $O(N^2Q + N^3 + N^2Q^2)$ to $O(\tilde{N}^2Q + \tilde{N}^3 + \tilde{N}^2Q^2)$. Note the critical role that our error bound plays in effecting this economy.

In practice — to ensure that the $\zeta_n, \hat{z}_0, \hat{z}_j^q$ are actually calculable — we replace the infinite-dimensional space Y with a very high-dimensional "truth" space Y_T (e.g., a finite element space associated with a very fine triangulation). It follows that we obtain bounds not for s, but rather for $s_T = \ell^O(u_T)$, where $u_T \in Y_T$ satisfies $a(u_T, v; \mu) = \ell(v), \forall v \in Y_T$. The essential point is that Y_T may be chosen very conservatively — and hence the difference between s_T and s rendered arbitrarily small — since (i) the on-line work and storage are in fact independent of the dimension of Y_T , \mathcal{N} , and (ii) the off-line work will remain modest since N will typically be quite small.

5 Results and Discussion

We first demonstrate the accuracy of the reduced-basis output prediction and output bounds by considering the case $P_{\rm eff}=5$ in which L=2.5 and t=0.25 are fixed; the remaining parameters k^1, k^2, k^3, k^4 , Bi vary in $\mathcal{D}_{\rm eff}\equiv [0.1, 10]^4\times [0.01, 1]$. The sample points for S^N are chosen randomly (uniformly) over $\mathcal{D}_{\rm eff}$; the new value of μ to which we apply the reduced-basis approximation is $k^1=0.5, k^2=1.0, k^3=3.0, k^4=9.0$, Bi = 0.6 (similar results are obtained at other points in $\mathcal{D}_{\rm eff}$). We present in Table 1 the actual error $|s(\mu)-s^N(\mu)|$; the estimated error $\Delta^N(\mu)$ (our strict upper bound for $|s(\mu)-s^N(\mu)|$); and the effectivity $\eta^N(\mu)$ (the ratio of the estimated and actual errors). We observe the high accuracy and rapid convergence of the reduced-basis prediction, even for this relatively high-dimensional parameter space; and the very good accuracy (low effectivity) of our error bound $\Delta^N(\mu)$. The combination of high accuracy and certifiable fidelity permits us to proceed with an extremely low number of modes.

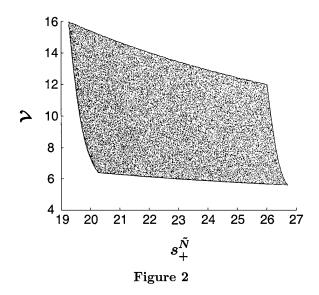
N	$ s-s^N $	Δ^N	η^N
10	4.68×10^{-3}	1.43×10^{-2}	3.06
20	4.70×10^{-4}	1.13×10^{-3}	2.40
30	3.04×10^{-4}	1.04×10^{-3}	3.43
40	1.08×10^{-4}	4.61×10^{-4}	4.27
50	2.47×10^{-5}	6.89×10^{-5}	2.78

Table 1

As regards computational cost, in the limit of "infinitely many" evaluations, the calculation of $\tilde{s}(\mu)$ to within 0.1% of s_T is roughly 24 times faster than direct calculation of $s_T = \ell^O(u_T)$; here u_T is our underlying "truth" finite element approximation. The breakeven point at which the reduced-basis approximation first becomes less expensive than direct evaluation of s_T is roughly 250 evaluations. These are fair comparisons: our "truth" approximation here is not overly fine, and our solution strategy for $u_T \in Y_T$ (an ILU-preconditioned conjugate-gradient procedure) is quite efficient. The reduced-basis approach is much faster simply because the dimension of W^N , N, is much smaller than the dimension of Y_T , \mathcal{N} (which more than compensates for the loss of sparsity in \underline{A}). For more difficult problems that require larger \mathcal{N} , or that are not as amenable to fast solution methods on Y_T , the relative efficiency of the reduced-basis approach is even more dramatic.

The obvious advantage of the reduced-basis approach within the design, optimization, and control environment is the very rapid response. However, the "blackbox" nature of the on-line component of the procedure has other advantages. In particular, the on-line code is simple, non-proprietary, and completely decoupled from the (often complicated) off-line "truth" code. This is particularly important in multidisciplinary design optimization, in which various models and approximations must be integrated.

We close this section with a more applied example. We now fix all parameters except L and t, so that $P_{\rm eff}=2$; (L,t) vary in $\mathcal{D}_{\rm eff}=[2.0,3.0]\times[0.1,0.5]$. We choose for our two outputs the volume of the fin, \mathcal{V} , and the root average temperature, s. As our "design exercise" we now construct the achievable set — all those (\mathcal{V},s) pairs associated with some (L,t) in $\mathcal{D}_{\rm eff}$; the result, based on many evaluations of $(\mathcal{V},s_+^{\tilde{N}})$ for different values of $(L,t)\in\mathcal{D}_{\rm eff}$, is shown in Figure 2. We present the results in terms of $s_+^{\tilde{N}}$ rather than $s_-^{\tilde{N}}$ to ensure that the actual temperature s_T will always be lower than our predictions (that is, conservative); and we choose \tilde{N} such that $s_+^{\tilde{N}}$ is always within 0.1% of s_T to ensure that the design process is not misled by inaccurate predictions. Given the obvious preferences of lower volume and lower temperature, the designer will be most interested in the lower left boundary of the achievable set — the Pareto efficient frontier; although this boundary can of course be found without constructing the entire achievable set, many evaluations of the outputs will still be required.



6 Generalizations and Issues

Many of the assumptions that we have introduced are assumptions of convenience and exposition, not necessity. First, the output functional ℓ^O need not be same as the inhomogeneity ℓ ; with the introduction of an adjoint (or dual) problem [2], our results above extend to the more general case. Second, the function $g(\mu)$ need not be known a priori: $g(\mu)$ is related to an eigenvalue problem which can itself be readily approximated by a reduced-basis space constructed as the span of appropriate eigenfunctions (in theory we can now only prove asymptotic bounding properties as $N \to \infty$, however in practice the reduced-basis eigenvalue approximation converges very rapidly, and there is thus little loss of certainty). Third, these same notions extend, with some modification, to noncoercive problems, where $g(\mu)$ is now in fact the inf-sup stability parameter [3, 4]. Finally, nonsymmetric operators are readily treated, as are certain classes of nonlinearity in the state variables (e.g., eigenvalue problems [1]).

Perhaps the most limiting assumption is (2), affine dependence on the parameter functions. In some cases (2) may indeed apply, but Q may be rather large. In such cases we can reduce the complexity and storage of the off-line and on-line stages from $O(Q^2)$ to O(Q) by introducing a reduced-basis approximation of the error equation (12) for a suitably chosen "staggered" sample set S_{err}^M and associated reduced-basis space constructed as the span of appropriate error functions. These ideas also extend to the case in which the parameter dependence can not be expressed (or accurately approximated) as in (2); however we now need to at least partially abandon the blackbox nature of the on-line stage of computation, allowing evaluation (though not inversion) of the truth-approximation operator, as well as storage of some reduced-basis vectors of size \mathcal{N} . These methods are currently under development.

References

- [1] L. Machiels, Y. Maday, I.B. Oliveira, A.T. Patera, and D.V. Rovas. Output bounds for reduced-basis approximations of symmetric positive definite eigenvalue problems. *C. R. Acad. Sci. Paris, Série I*, to appear.
- [2] L. MACHIELS, Y. MADAY, A.T. PATERA, AND D.V. ROVAS. Blackbox reduced-basis output bound methods for shape optimization. In *Proceedings* 12th International Domain Decomposition Conference, Chiba Japan, 2000, to appear.
- [3] D.V. Rovas. An overview of blackbox reduced-basis output bound methods for elliptic partial differential equations. In *Proceedings* 16th IMACS World Congress 2000, Lausanne Switzerland, 2000, to appear.
- [4] Y. Maday, A.T. Patera, and D.V. Rovas. A blackbox reduced-basis output bound method for noncoercive linear problems. *MIT-FML Report* 00-2-1, 2000; also in the Collège de France Series, to appear.
- [5] A.K. NOOR AND J.M. PETERS. Reduced basis technique for nonlinear analysis of structures. *AIAA Journal*, 18(4):455-462, 1980.
- [6] J.P. Fink and W.C. Rheinboldt. On the error behavior of the reduced basis technique in nonlinear finite element approximations. Z. Angew. Math. Mech., 63:21-28, 1983.
- [7] T.A. PORSCHING. Estimation of the error in the reduced basis method solution of nonlinear equations. *Mathematics of Computation*, 45(172):487-496, 1985.
- [8] Y. MADAY, A.T. PATERA, AND J. PERAIRE. A general formulation for a posteriori bounds for output functionals of partial differential equations; application to the eigenvalue problem. C. R. Acad. Sci. Paris, Série I, 328:823-829, 1999.
- [9] A.T. PATERA AND E.M. RØNQUIST. A general output bound result: application to discretization and iteration error estimation and control. *Math. Models Methods Appl. Sci.*, to appear.

Personnel Supported

Faculty: Anthony T. Patera

Post-Docs: Luc Machiels

Graduate Students: Thomas B. Leurent

Ivan B. Oliveira Dimitrios V. Rovas Jeremy Teichman

Other: None

Publications

M. Paraschivoiu, J. Peraire, and A.T. Patera. A posteriori finite element bounds for linear-functional outputs of elliptic partial differential equations. Comput. Methods Appl. Mech. Engrg. 150:289-312, 1997.

- J. Peraire and A.T. Patera. Bounds for linear-functional outputs of coercive partial differential equations: local indicators and adaptive refinement. Advances in Adaptive Computational Methods in Mechanics, eds. P. Ladevèze and J.T. Oden, 1998, pp. 199–216.
- L. Machiels, A.T. Patera, J. Peraire, and Y. Maday. A general framework for finite element a posteriori error control: application to linear and nonlinear convection-dominated problems. Presented at ICFD Conference on Numerical Methods for Fluid Dynamics, Oxford, England, March 31 – April 3, 1998.
- L. Machiels, J. Peraire, and A.T. Patera. Output bound approximations for partial differential equations; application to the incompressible Navier– Stokes equations. *Industrial and Environmental Applications of Direct and Large-Eddy Simulations*, eds. S. Biringen, H. Örs, A. Tezel, J.H. Ferziger, pp. 93–108, 1998.
- Y. Maday, A.T. Patera, and J. Peraire. A general formulation for a posteriori bounds for output functionals of partial differential equations; application to the eigenvalue problem. C.R. Acad. Sci. Paris Série I, 328: 823–828, 1999.
- J. Sarrate, J. Peraire, and A.T. Patera. A posteriori finite element error bounds for non-linear outputs of the Helmholtz equation. Int. J. Numer. Meth. Fluids, 31:17–36, 1999.
- D.V. Rovas and A.T. Patera. Reduced-basis output-bound methods for elliptic partial differential equations. 2nd ISSMO/AIAA Internet Conference on Approximations and Fast Reanalysis in Engineering Optimization, May 25 June 2, 2000.

- L. Machiels, Y. Maday, and A.T. Patera. A "flux-free" nodal Neumann subproblem approach to output bounds for partial differential equations. *C.R. Acad. Sci. Paris*, Série I, **330**:249–254, 2000.
- M. Paraschivoiu and A.T. Patera. A posteriori bounds for linear functional outputs of Crouzeix-Raviart finite element discretizations of the incompressible Stokes problem. Int. J. Numer. Meth. Fluids, 32:823-849, 2000.
- L. Machiels, Y. Maday, I.B. Oliveira, A.T. Patera, and D.V. Rovas. Output bounds for reduced-basis approximations of symmetric positive definite eigenvalue problems. C. R. Acad. Sci. Paris, Série I, to appear.
- L. Machiels, Y. Maday, A.T. Patera, and D.V. Rovas. Blackbox reduced-basis output bound method for shape optimization. In *Proceedings* 12th *International Domain Decomposition Conference*, Chiba Japan, 2000, to appear.
- L. Machiels, Y. Maday, and A.T. Patera. Output bounds for reduced-order approximations of elliptic partial differential equations. *Comput. Methods Appl. Mech. Engrg.*, to appear.
- D.V. Rovas. An overview of blackbox reduced-basis output bound methods for elliptic partial differential equations. In *Proceedings* 16th *IMACS World Congress* 2000, Lausanne Switzerland, 2000, to appear.
- A.T. Patera. Output bounds for elliptic partial differential equations: a general formulation. In *Proceedings* 16th *IMACS World Congress* 2000, Lausanne Switzerland, 2000, to appear.
- Y. Maday, A.T. Patera, and D.V. Rovas. A blackbox reduced-basis output bound method for noncoercive linear problems. *Nonlinear Partial Differential Equations and Their Applications, Collège de France Series*, to appear.
- A.T. Patera and E.M. Rönquist. A general output bound result: application to discretization and iteration error estimation and control. *Mathematical Models and Methods in Applied Sciences*, to appear.
- L. Machiels, J. Peraire, and A.T. Patera. A posteriori finite element output bounds for the incompressible Navier–Stokes equations; application to a natural convection problem. Journal of Computational Physics, submitted.